



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 01:31 PM EDT

PDB ID : 5GW4
EMDB ID: : EMD-9540
Title : Structure of Yeast NPP-TRiC
Authors : Zang, Y.; Jin, M.; Wang, H.; Cong, Y.
Deposited on : 2016-09-08
Resolution : 4.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

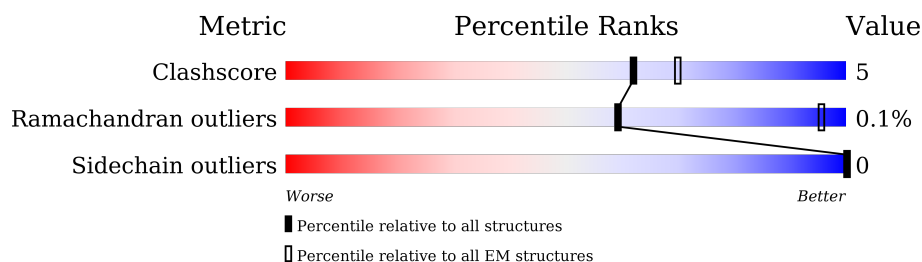
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




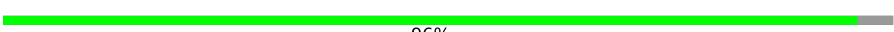

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	559	
1	a	559	
2	B	527	
2	b	527	
3	D	528	
3	d	528	
4	E	562	
4	e	562	
5	G	534	

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Mol	Chain	Length	Quality of chain
5	g	534	 97% .
6	H	550	 69% 25% 6%
6	h	550	 94% 6%
7	Q	568	 74% 22% .
7	q	568	 96% .
8	Z	546	 73% 25% .
8	z	546	 98% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 64544 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	543	Total	C	N	O	S	0	0
			4103	2566	717	800	20		
1	A	543	Total	C	N	O	S	0	0
			4103	2566	717	800	20		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	517	Total	C	N	O	S	0	0
			3930	2456	679	781	14		
2	B	517	Total	C	N	O	S	0	0
			3930	2456	679	781	14		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	521	Total	C	N	O	S	0	0
			3985	2484	709	775	17		
3	D	521	Total	C	N	O	S	0	0
			3985	2484	709	775	17		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	528	Total	C	N	O	S	0	0
			4068	2550	699	798	21		
4	E	528	Total	C	N	O	S	0	0
			4068	2550	699	798	21		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	518	Total	C	N	O	S	0	0
			3982	2496	696	764	26		
5	G	518	Total	C	N	O	S	0	0
			3982	2496	696	764	26		

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	519	Total	C	N	O	S	0	0
			3969	2501	678	771	19		
6	H	519	Total	C	N	O	S	0	0
			3969	2501	678	771	19		

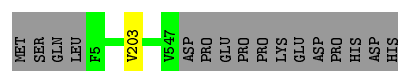
- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	543	Total	C	N	O	S	0	0
			4125	2598	703	798	26		
7	Q	543	Total	C	N	O	S	0	0
			4125	2598	703	798	26		

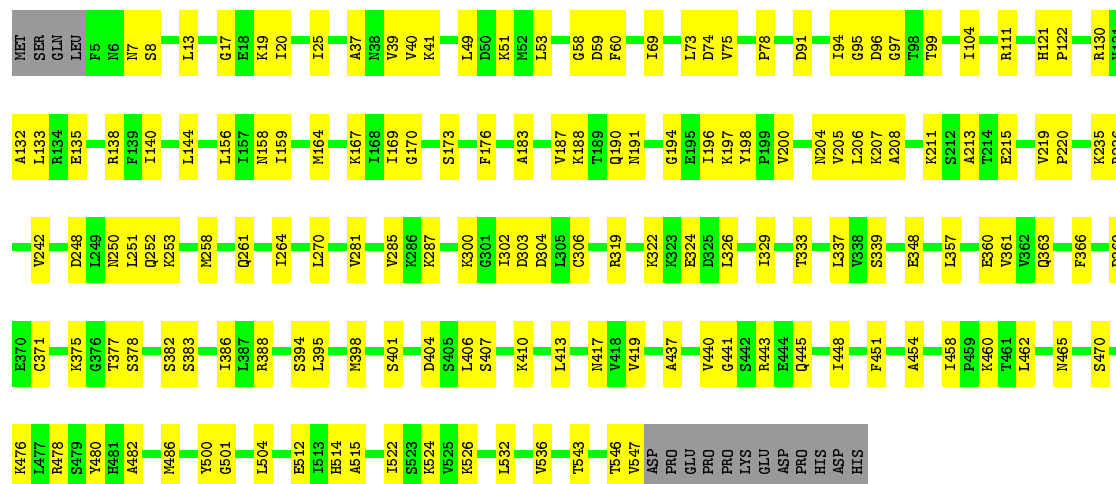
- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	534	Total	C	N	O	S	0	0
			4110	2582	712	799	17		
8	Z	534	Total	C	N	O	S	0	0
			4110	2582	712	799	17		

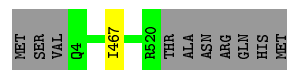
- Molecule 1: T-complex protein 1 subunit alpha



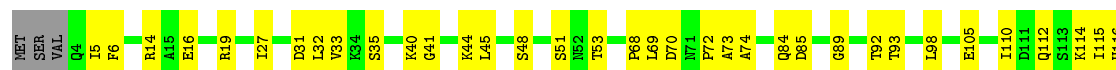
- Chain A: 70% 28% .

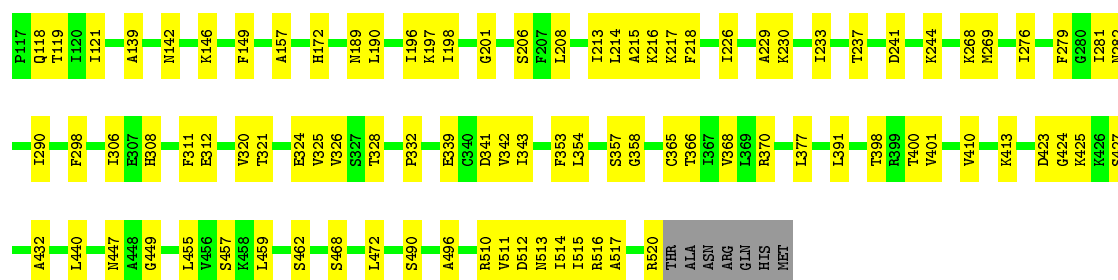


- Chain b:  98%

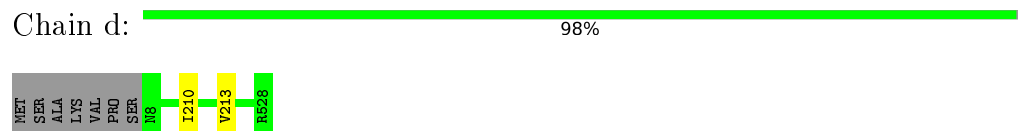


- Chain B:  74% 24%

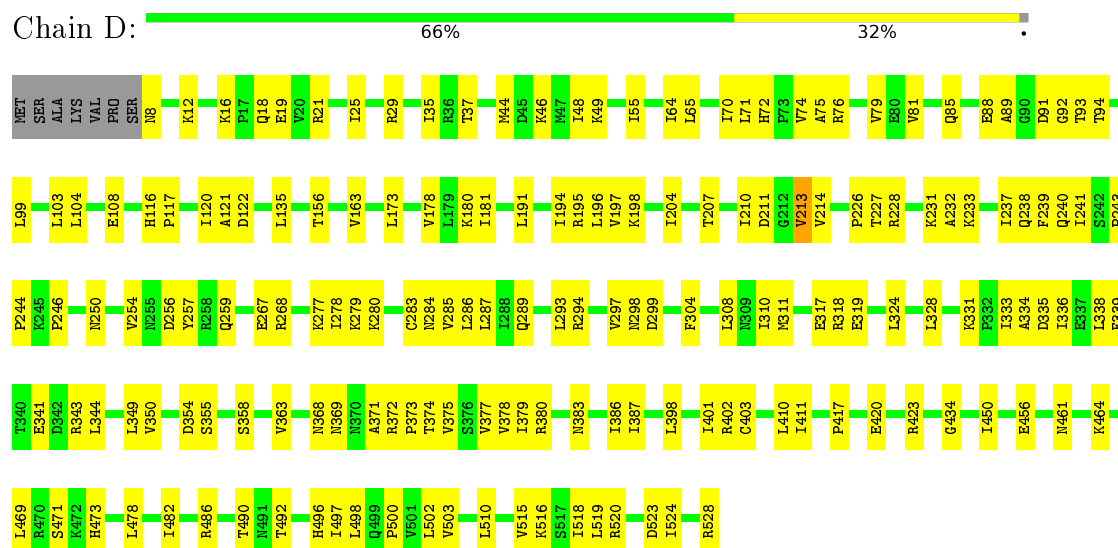




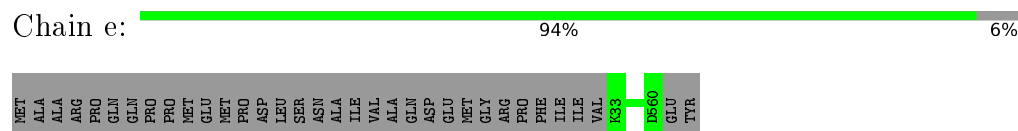
- Molecule 3: T-complex protein 1 subunit delta



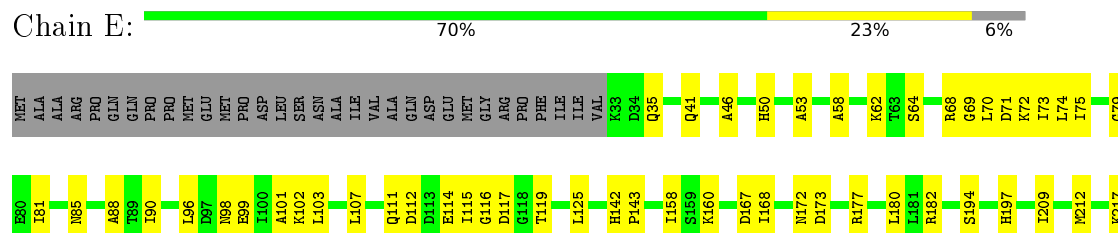
- Molecule 3: T-complex protein 1 subunit delta

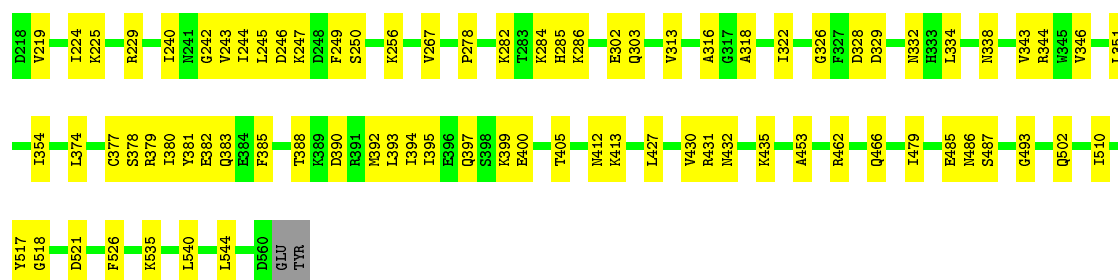


- Molecule 4: T-complex protein 1 subunit epsilon



- Molecule 4: T-complex protein 1 subunit epsilon





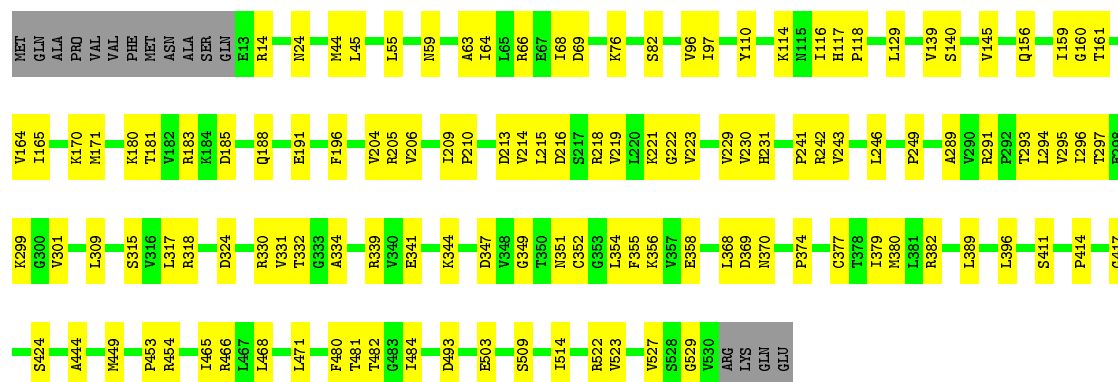
- Molecule 5: T-complex protein 1 subunit gamma

Chain g: 97%



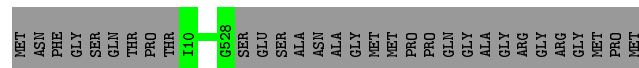
- Molecule 5: T-complex protein 1 subunit gamma

Chain G: 74%



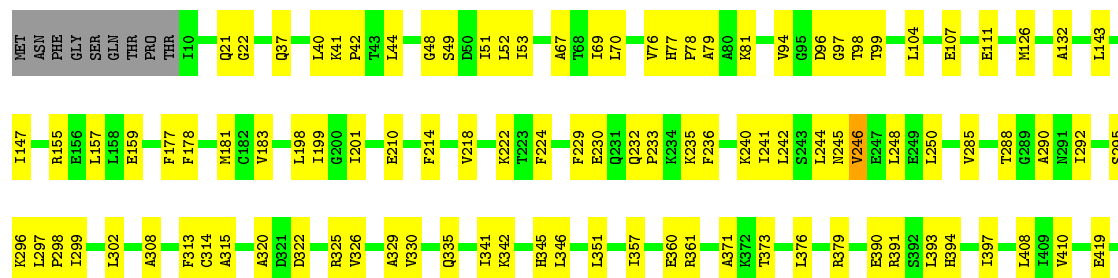
- Molecule 6: T-complex protein 1 subunit eta

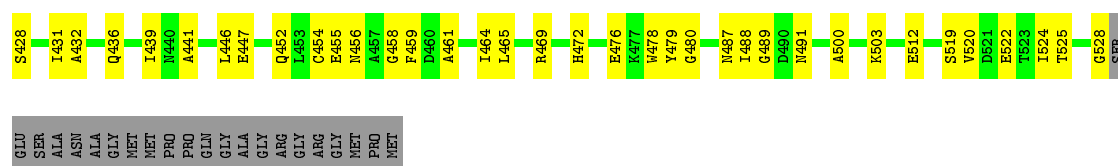
Chain h: 94%



- Molecule 6: T-complex protein 1 subunit eta

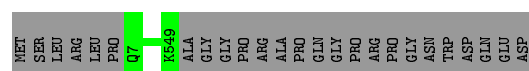
Chain H: 69%





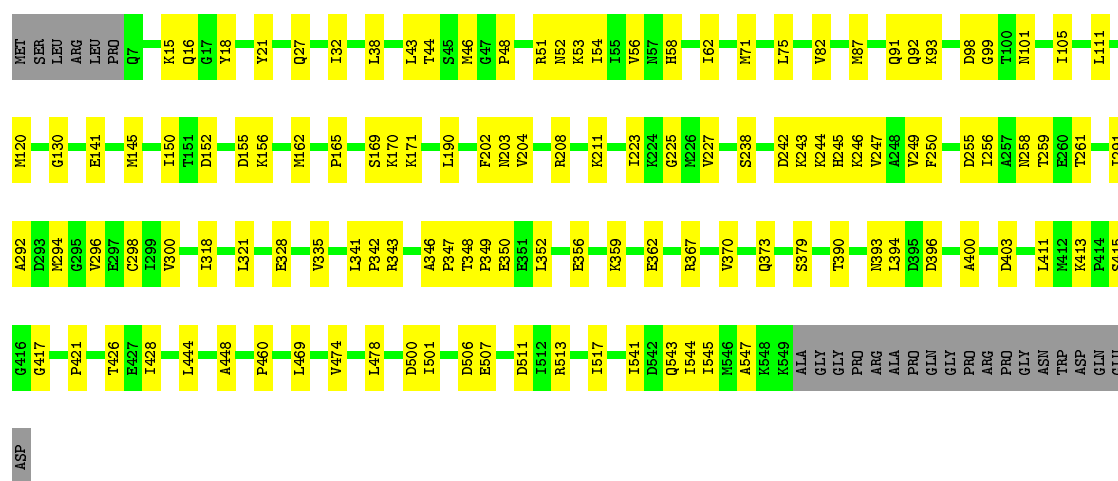
- Molecule 7: T-complex protein 1 subunit theta

Chain q: 96%



- Molecule 7: T-complex protein 1 subunit theta

Chain Q: 74% 22%



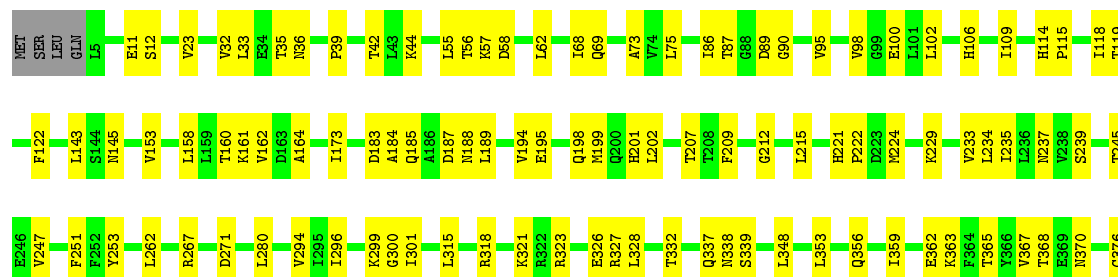
- Molecule 8: T-complex protein 1 subunit zeta

Chain z: 98%



- Molecule 8: T-complex protein 1 subunit zeta

Chain Z: 73% 25%



R538	L379
SER	L380
THR	K381
LEU	G382
LYS	S383
GLU	T384
THR	L388
PRO	D393
GLN	R396
	D397
	R400
	A403
	P404
	V405
	L406
	K407
	S423
	K437
	T440
	L451
	L452
	V453
	V459
	V469
	G490
	V491
	D492
	C499
	R511
	V512
	T521
	G522
	I523
	A524
	S525
	L529
	G530
	D531
	E532
	R535
	A536
	E537

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	107318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	18000	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.23	0/4140	0.41	0/5585
1	a	0.23	0/4140	0.40	0/5585
2	B	0.23	0/3969	0.40	0/5348
2	b	0.23	0/3969	0.40	0/5348
3	D	0.23	0/4022	0.40	0/5421
3	d	0.23	0/4022	0.39	0/5421
4	E	0.23	0/4117	0.39	0/5539
4	e	0.23	0/4117	0.39	0/5539
5	G	0.23	0/4029	0.39	0/5442
5	g	0.23	0/4029	0.38	0/5442
6	H	0.23	0/4018	0.39	0/5422
6	h	0.23	0/4018	0.38	0/5422
7	Q	0.25	1/4175 (0.0%)	0.41	0/5636
7	q	0.24	0/4175	0.40	0/5636
8	Z	0.23	0/4162	0.39	0/5624
8	z	0.23	0/4162	0.40	0/5624
All	All	0.23	1/65264 (0.0%)	0.40	0/88034

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	346	ALA	C-N	5.67	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	H	246	VAL	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4103	0	4269	108	0
1	a	4103	0	4269	0	0
2	B	3930	0	4034	85	0
2	b	3930	0	4034	0	0
3	D	3985	0	4157	119	0
3	d	3985	0	4157	0	0
4	E	4068	0	4163	101	0
4	e	4068	0	4163	0	0
5	G	3982	0	4123	93	0
5	g	3982	0	4123	0	0
6	H	3969	0	4055	96	0
6	h	3969	0	4055	0	0
7	Q	4125	0	4260	90	0
7	q	4125	0	4260	0	0
8	Z	4110	0	4204	96	0
8	z	4110	0	4204	0	0
All	All	64544	0	66530	714	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:212:GLY:H	8:Z:368:THR:HG22	1.50	0.77
4:E:380:ILE:HG12	4:E:395:ILE:HG12	1.72	0.74
3:D:289:GLN:HE21	3:D:318:ARG:HG2	1.70	0.73
6:H:42:PRO:HB2	6:H:49:SER:HB2	1.71	0.73
8:Z:36:ASN:HA	8:Z:42:THR:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASN:HB3	1:A:300:LYS:HB2	1.70	0.72
5:G:243:VAL:H	5:G:349:GLY:HA3	1.55	0.71
2:B:197:LYS:HD2	2:B:377:LEU:HB3	1.73	0.71
7:Q:21:TYR:HB3	7:Q:27:GLN:HG2	3.92	0.71
4:E:247:LYS:HE2	4:E:344:ARG:H	1.69	0.71
6:H:22:GLY:H	6:H:522:GLU:HG2	6.31	0.70
5:G:222:GLY:HA2	5:G:331:VAL:HG11	1.71	0.70
3:D:121:ALA:HB1	3:D:516:LYS:HG3	2.40	0.70
2:B:214:LEU:HB2	2:B:354:LEU:HB2	1.74	0.70
3:D:232:ALA:HA	3:D:284:ASN:HD22	1.57	0.70
5:G:206:VAL:HG12	5:G:379:ILE:HB	1.75	0.69
6:H:520:VAL:HB	7:Q:51:ARG:HD3	8.18	0.69
5:G:466:ARG:HA	7:Q:444:LEU:HD21	60.29	0.69
3:D:89:ALA:HB1	3:D:503:VAL:HG22	1.82	0.68
6:H:241:ILE:HA	6:H:292:ILE:HB	2.24	0.68
4:E:194:SER:O	4:E:197:HIS:ND1	2.27	0.67
4:E:240:ILE:HG22	4:E:242:GLY:H	1.73	0.67
1:A:40:VAL:HB	1:A:99:THR:HG23	1.74	0.67
2:B:119:THR:OG1	4:E:68:ARG:NH2	2.27	0.67
4:E:247:LYS:HG3	4:E:343:VAL:HG13	3.79	0.67
6:H:246:VAL:HG11	6:H:297:LEU:HD12	1.75	0.67
5:G:230:VAL:HG11	5:G:318:ARG:HG2	1.98	0.67
5:G:242:ARG:HA	5:G:349:GLY:HA3	2.99	0.66
1:A:501:GLY:HA3	1:A:512:GLU:HG2	1.75	0.66
1:A:407:SER:HA	1:A:410:LYS:HE2	1.77	0.66
7:Q:165:PRO:HB3	7:Q:517:ILE:HG23	2.15	0.65
4:E:68:ARG:NH1	4:E:486:ASN:O	2.27	0.65
6:H:322:ASP:OD1	6:H:325:ARG:NH2	2.29	0.65
1:A:167:LYS:HD3	1:A:401:SER:HB2	5.52	0.65
4:E:41:GLN:HB3	4:E:46:ALA:HB2	2.37	0.64
7:Q:428:ILE:HD11	7:Q:460:PRO:HG3	1.80	0.64
8:Z:393:ASP:OD1	8:Z:396:ARG:NH2	2.30	0.64
1:A:261:GLN:HB2	5:G:289:ALA:HA	1.79	0.64
8:Z:221:HIS:HB3	8:Z:224:MET:HG2	3.33	0.64
1:A:140:ILE:HG22	1:A:144:LEU:HD23	4.05	0.64
4:E:388:THR:HG22	4:E:390:ASP:H	1.63	0.64
6:H:519:SER:HB2	7:Q:51:ARG:HD2	3.25	0.64
8:Z:367:VAL:O	8:Z:370:ASN:ND2	2.30	0.64
5:G:249:PRO:HB3	5:G:299:LYS:HB2	1.87	0.64
6:H:297:LEU:HB3	6:H:298:PRO:HD2	1.80	0.63
8:Z:161:LYS:NZ	8:Z:397:ASP:OD2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:476:GLU:HG3	6:H:478:TRP:H	1.63	0.63
7:Q:227:VAL:HG13	7:Q:370:VAL:HG12	2.51	0.63
1:A:264:ILE:HG21	1:A:270:LEU:HB2	1.80	0.63
1:A:200:VAL:HA	1:A:410:LYS:HD3	2.95	0.63
5:G:215:LEU:O	5:G:218:ARG:NH1	2.28	0.63
7:Q:15:LYS:HG2	8:Z:68:ILE:HG12	1.80	0.63
1:A:478:ARG:HH11	6:H:436:GLN:HE21	130.16	0.63
7:Q:170:LYS:HD2	7:Q:400:ALA:HB2	1.79	0.63
4:E:115:ILE:HG12	4:E:432:ASN:HD21	4.58	0.62
8:Z:237:ASN:HB3	8:Z:338:ASN:HA	1.81	0.62
4:E:217:LYS:HD3	4:E:435:LYS:HA	1.80	0.62
8:Z:397:ASP:OD1	8:Z:400:ARG:NH2	2.31	0.62
6:H:155:ARG:HA	6:H:183:VAL:HG11	1.81	0.62
2:B:233:ILE:HG21	2:B:325:VAL:HG12	1.81	0.62
3:D:198:LYS:HB2	3:D:387:ILE:HB	4.31	0.62
6:H:147:ILE:HD11	6:H:157:LEU:HD13	1.81	0.62
6:H:244:LEU:HD21	6:H:341:ILE:HD11	1.82	0.62
8:Z:300:GLY:HA2	8:Z:318:ARG:HB2	1.81	0.62
5:G:243:VAL:HG13	5:G:296:ILE:HD12	1.82	0.62
3:D:331:LYS:HD3	3:D:343:ARG:HE	3.50	0.62
3:D:254:VAL:HG13	3:D:259:GLN:HB2	3.74	0.61
6:H:199:ILE:HG21	6:H:397:ILE:HG21	4.16	0.61
3:D:88:GLU:O	3:D:402:ARG:NH2	2.73	0.61
6:H:487:ASN:OD1	6:H:488:ILE:N	2.34	0.61
6:H:198:LEU:O	6:H:373:THR:OG1	2.19	0.61
7:Q:44:THR:OG1	7:Q:53:LYS:NZ	2.32	0.61
2:B:139:ALA:HA	2:B:401:VAL:HG12	1.82	0.61
5:G:216:ASP:O	5:G:382:ARG:NH2	2.29	0.61
2:B:33:VAL:HB	2:B:93:THR:HG23	2.51	0.61
7:Q:52:ASN:ND2	7:Q:396:ASP:OD2	5.13	0.61
1:A:248:ASP:HB3	1:A:339:SER:HA	2.69	0.60
3:D:246:PRO:HD2	3:D:250:ASN:HD22	1.81	0.60
4:E:35:GLN:HB2	6:H:76:VAL:HG21	8.03	0.60
2:B:230:LYS:NZ	2:B:339:GLU:OE1	2.33	0.60
8:Z:323:ARG:HG3	8:Z:327:ARG:HH12	1.66	0.60
2:B:510:ARG:O	4:E:71:ASP:N	2.34	0.60
6:H:201:ILE:HG12	6:H:376:LEU:HB3	1.96	0.60
6:H:428:SER:HB2	6:H:436:GLN:HG3	1.84	0.60
7:Q:243:LYS:HE2	7:Q:244:LYS:HE3	7.18	0.59
3:D:238:GLN:HB2	3:D:334:ALA:HA	2.84	0.59
3:D:411:ILE:HG23	3:D:478:LEU:HD11	5.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:172:ASN:OD1	4:E:173:ASP:N	2.35	0.59
4:E:125:LEU:HB2	4:E:479:ILE:HD11	1.84	0.59
2:B:462:SER:O	2:B:468:SER:OG	2.19	0.59
1:A:135:GLU:OE1	1:A:138:ARG:NH2	3.00	0.59
2:B:279:PHE:HE1	2:B:332:PRO:HA	1.67	0.59
1:A:546:THR:HG23	3:D:49:LYS:HD3	1.85	0.59
3:D:25:ILE:HG23	3:D:104:LEU:HB3	1.93	0.59
6:H:240:LYS:HB2	6:H:290:ALA:HA	1.89	0.59
7:Q:300:VAL:HG22	7:Q:321:LEU:HD23	1.90	0.59
2:B:269:MET:SD	4:E:172:ASN:ND2	2.75	0.59
4:E:103:LEU:HB3	4:E:544:LEU:HD11	1.83	0.59
5:G:241:PRO:HG3	5:G:355:PHE:HB2	2.93	0.59
8:Z:143:LEU:HG	8:Z:145:ASN:H	1.68	0.59
6:H:126:MET:SD	6:H:519:SER:OG	4.65	0.59
2:B:110:ILE:O	2:B:114:LYS:N	2.35	0.58
4:E:510:ILE:HG23	4:E:521:ASP:H	1.80	0.58
8:Z:229:LYS:HA	8:Z:353:LEU:HA	1.85	0.58
2:B:208:LEU:HD11	2:B:365:CYS:HB2	1.84	0.58
5:G:331:VAL:HG12	5:G:374:PRO:HG3	1.85	0.58
5:G:482:THR:HA	5:G:493:ASP:HA	2.25	0.58
7:Q:243:LYS:HG2	7:Q:244:LYS:HG3	5.09	0.58
3:D:233:LYS:NZ	3:D:341:GLU:OE2	2.36	0.58
3:D:198:LYS:HB3	3:D:387:ILE:HD12	1.84	0.58
3:D:471:SER:HB3	4:E:462:ARG:HD2	119.34	0.58
4:E:68:ARG:HD3	4:E:487:SER:HA	1.85	0.58
2:B:198:ILE:HD11	2:B:370:ARG:HG2	1.85	0.58
2:B:51:SER:O	3:D:76:ARG:NH1	2.38	0.58
4:E:115:ILE:HG22	4:E:117:ASP:H	1.74	0.58
7:Q:162:MET:HG2	7:Q:411:LEU:HD21	1.85	0.58
4:E:88:ALA:HB2	4:E:119:THR:HG21	1.84	0.58
5:G:160:GLY:HA2	5:G:165:ILE:HD13	4.49	0.58
7:Q:343:ARG:NH2	8:Z:253:TYR:OH	2.36	0.58
1:A:121:HIS:NE2	3:D:456:GLU:O	2.37	0.58
2:B:226:ILE:HB	2:B:343:ILE:HB	1.85	0.58
2:B:197:LYS:HB3	2:B:377:LEU:HD13	1.87	0.58
6:H:241:ILE:HG13	6:H:330:VAL:HG11	1.86	0.58
2:B:112:GLN:HA	3:D:12:LYS:HG3	22.85	0.58
6:H:233:PRO:HG2	6:H:236:PHE:HE1	1.84	0.58
6:H:218:VAL:HG11	6:H:326:VAL:HG22	2.83	0.58
8:Z:323:ARG:NH1	8:Z:326:GLU:OE1	2.37	0.57
6:H:431:ILE:HG21	6:H:439:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:231:LYS:O	3:D:284:ASN:ND2	2.38	0.57
6:H:132:ALA:HB2	6:H:439:ILE:HG12	1.87	0.57
3:D:383:ASN:H	3:D:386:ILE:HD12	1.70	0.57
4:E:114:GLU:O	4:E:431:ARG:NH2	2.37	0.57
6:H:78:PRO:HB2	7:Q:54:ILE:HD13	1.86	0.57
5:G:209:ILE:HD12	5:G:380:MET:HG3	1.84	0.57
1:A:156:LEU:HD23	1:A:159:ILE:HD12	1.85	0.57
1:A:251:LEU:HD12	1:A:302:ILE:HG12	2.26	0.57
6:H:525:THR:HA	7:Q:56:VAL:HB	1.84	0.57
8:Z:56:THR:HG22	8:Z:58:ASP:H	1.69	0.57
3:D:194:ILE:HG12	3:D:375:VAL:HB	3.15	0.57
3:D:372:ARG:HB2	3:D:373:PRO:HD2	1.85	0.57
1:A:187:VAL:HG22	1:A:382:SER:HA	1.87	0.57
1:A:253:LYS:HA	1:A:281:VAL:HG11	1.85	0.57
3:D:279:LYS:HB2	3:D:308:LEU:HD23	1.86	0.57
4:E:313:VAL:HG13	4:E:318:ALA:HB3	1.86	0.57
8:Z:221:HIS:HB3	8:Z:224:MET:HG3	1.86	0.57
7:Q:150:ILE:HG22	7:Q:152:ASP:H	1.70	0.56
8:Z:185:GLN:HG3	8:Z:187:ASP:HB2	1.86	0.56
1:A:242:VAL:HG11	1:A:361:VAL:HG23	2.07	0.56
8:Z:162:VAL:HG23	8:Z:164:ALA:H	1.77	0.56
4:E:180:LEU:HD22	4:E:430:VAL:HG13	3.80	0.56
3:D:65:LEU:HB3	3:D:79:VAL:HG22	1.87	0.56
2:B:69:LEU:HD13	2:B:74:ALA:HB1	1.87	0.56
8:Z:153:VAL:HG11	8:Z:405:VAL:HG21	1.93	0.56
3:D:71:LEU:HA	3:D:76:ARG:HH21	1.70	0.56
1:A:476:LYS:HG2	6:H:432:ALA:HB1	130.92	0.56
7:Q:211:LYS:HB2	7:Q:394:LEU:HD21	4.60	0.56
6:H:250:LEU:HD12	6:H:302:LEU:HD22	1.88	0.56
6:H:410:VAL:HG13	6:H:500:ALA:HB2	1.87	0.56
7:Q:48:PRO:HA	7:Q:169:SER:HA	1.88	0.56
6:H:44:LEU:HD23	6:H:452:GLN:HB2	1.91	0.56
6:H:53:ILE:HD11	6:H:69:ILE:HG23	1.96	0.56
2:B:324:GLU:HG3	2:B:326:VAL:HG22	6.53	0.56
1:A:211:LYS:HB2	1:A:388:ARG:HD3	6.13	0.55
5:G:96:VAL:HG22	5:G:509:SER:HA	1.88	0.55
8:Z:100:GLU:HG2	8:Z:453:VAL:HB	1.88	0.55
1:A:251:LEU:HB2	1:A:302:ILE:HG12	1.88	0.55
1:A:158:ASN:ND2	1:A:514:HIS:O	2.34	0.55
3:D:411:ILE:HD12	3:D:417:PRO:HG3	1.88	0.55
2:B:425:LYS:HD3	3:D:8:ASN:HB3	41.01	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:246:LYS:HB2	7:Q:296:VAL:HA	2.41	0.55
5:G:55:LEU:HD11	8:Z:75:LEU:HD21	1.87	0.55
3:D:355:SER:HB2	3:D:358:SER:HB2	4.11	0.55
3:D:191:LEU:HG	3:D:402:ARG:HD3	1.87	0.55
3:D:298:ASN:OD1	3:D:299:ASP:N	2.39	0.55
6:H:222:LYS:HE2	6:H:360:GLU:HG3	2.51	0.55
6:H:408:LEU:HG	6:H:500:ALA:HB3	1.89	0.55
7:Q:543:GLN:HE21	7:Q:545:ILE:HD11	3.44	0.55
3:D:277:LYS:HA	3:D:280:LYS:HD3	4.20	0.55
1:A:287:LYS:HG3	1:A:348:GLU:HA	1.88	0.55
2:B:19:ARG:NH2	3:D:8:ASN:O	34.97	0.55
4:E:243:VAL:HG11	4:E:354:ILE:HG12	1.89	0.55
4:E:75:ILE:HG12	4:E:81:ILE:HG12	2.75	0.55
1:A:235:LYS:HB3	1:A:363:GLN:HB3	2.04	0.55
1:A:451:PHE:HE1	1:A:532:LEU:HD11	1.72	0.55
4:E:244:ILE:HG23	4:E:245:LEU:H	4.09	0.55
5:G:180:LYS:HG2	5:G:183:ARG:HH21	1.72	0.55
1:A:13:LEU:HD21	1:A:19:LYS:HD3	2.20	0.54
1:A:220:PRO:HD2	1:A:375:LYS:HE2	1.89	0.54
5:G:205:ARG:NH2	5:G:324:ASP:OD1	2.40	0.54
5:G:219:VAL:HG13	5:G:379:ILE:HG12	1.89	0.54
4:E:142:HIS:NE2	6:H:455:GLU:O	2.40	0.54
1:A:215:GLU:O	1:A:388:ARG:NH2	2.36	0.54
2:B:520:ARG:HH21	4:E:79:GLY:HA3	1.71	0.54
5:G:183:ARG:NH1	5:G:185:ASP:OD2	2.40	0.54
6:H:480:GLY:N	6:H:489:GLY:O	2.39	0.54
3:D:368:ASN:HB3	3:D:371:ALA:HB3	1.90	0.54
5:G:159:ILE:HG23	5:G:164:VAL:HG23	2.41	0.54
3:D:333:ILE:HD13	3:D:339:PHE:HA	4.57	0.54
8:Z:36:ASN:HD21	8:Z:44:LYS:HD2	3.78	0.54
2:B:311:PHE:CE1	2:B:312:GLU:HG3	2.45	0.54
2:B:40:LYS:NZ	3:D:122:ASP:OD2	2.41	0.54
5:G:206:VAL:HG22	5:G:379:ILE:HB	5.20	0.54
1:A:252:GLN:HA	1:A:303:ASP:HB2	1.90	0.54
8:Z:33:LEU:HD12	8:Z:95:VAL:HG11	1.88	0.54
5:G:45:LEU:HD23	5:G:59:ASN:HB3	1.89	0.54
6:H:48:GLY:HA2	6:H:456:ASN:HB3	2.23	0.54
3:D:278:ILE:HG21	3:D:286:LEU:HD11	1.89	0.54
5:G:181:THR:HG23	5:G:221:LYS:HG2	1.89	0.54
6:H:40:LEU:HD11	6:H:70:LEU:HD21	2.48	0.54
6:H:528:GLY:HA3	7:Q:58:HIS:HA	3.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:194:VAL:HG22	8:Z:376:CYS:HB2	2.26	0.54
7:Q:16:GLN:HB2	7:Q:18:TYR:CE2	2.43	0.53
7:Q:249:VAL:HA	7:Q:300:VAL:HB	2.30	0.53
7:Q:56:VAL:HG22	7:Q:62:ILE:HG12	1.90	0.53
7:Q:87:MET:HE2	8:Z:384:THR:HB	4.89	0.53
8:Z:32:VAL:O	8:Z:44:LYS:NZ	3.06	0.53
1:A:39:VAL:HG12	1:A:51:LYS:HZ2	3.95	0.53
2:B:215:ALA:HA	2:B:353:PHE:HA	1.90	0.53
4:E:284:LYS:HG2	4:E:286:LYS:H	4.60	0.53
5:G:242:ARG:N	5:G:293:THR:OG1	2.41	0.53
6:H:81:LYS:HD3	7:Q:62:ILE:HD12	1.91	0.53
1:A:190:GLN:HB3	1:A:194:GLY:HA2	2.15	0.53
3:D:284:ASN:O	3:D:311:MET:N	2.44	0.53
3:D:135:LEU:HD11	3:D:411:ILE:HD13	1.89	0.53
5:G:351:ASN:O	5:G:370:ASN:ND2	3.83	0.53
7:Q:259:THR:HG22	7:Q:261:THR:H	1.78	0.53
7:Q:247:VAL:HG22	7:Q:298:CYS:HB3	1.90	0.53
3:D:334:ALA:H	3:D:338:LEU:HD23	4.58	0.53
4:E:96:LEU:HD13	4:E:98:ASN:HB2	3.02	0.53
5:G:331:VAL:HG23	5:G:332:THR:HG23	1.90	0.53
8:Z:321:LYS:HE2	8:Z:323:ARG:HB2	2.80	0.53
1:A:333:THR:HG22	1:A:377:THR:HG21	1.90	0.53
2:B:70:ASP:O	2:B:516:ARG:NH1	9.10	0.53
8:Z:459:VAL:HG11	8:Z:469:VAL:HG21	4.19	0.53
2:B:73:ALA:HB2	2:B:514:ILE:HD13	1.91	0.53
6:H:77:HIS:HE1	6:H:79:ALA:HB3	1.95	0.53
1:A:53:LEU:HD11	1:A:69:ILE:HG12	1.91	0.52
1:A:17:GLY:HA3	1:A:547:VAL:HA	2.07	0.52
8:Z:337:GLN:NE2	8:Z:339:SER:O	2.88	0.52
3:D:523:ASP:OD1	3:D:524:ILE:N	2.42	0.52
4:E:224:ILE:HD13	4:E:427:LEU:HD13	1.90	0.52
7:Q:506:ASP:OD1	7:Q:507:GLU:N	3.50	0.52
2:B:146:LYS:HA	2:B:149:PHE:HB3	2.12	0.52
3:D:285:VAL:HG22	3:D:311:MET:HB3	1.90	0.52
4:E:158:ILE:HD13	4:E:535:LYS:HE3	1.93	0.52
4:E:247:LYS:HB2	4:E:393:LEU:HD23	3.74	0.52
6:H:229:PHE:HE2	6:H:361:ARG:HD2	1.74	0.52
6:H:51:ILE:HD12	6:H:69:ILE:HD13	2.15	0.52
2:B:214:LEU:HD11	2:B:354:LEU:HD12	5.18	0.52
2:B:85:ASP:HA	2:B:89:GLY:HA2	1.92	0.52
4:E:247:LYS:HG3	4:E:249:PHE:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:322:ILE:HA	4:E:343:VAL:HB	2.22	0.52
4:E:412:ASN:OD1	4:E:413:LYS:N	2.42	0.52
5:G:454:ARG:HH22	7:Q:120:MET:HA	57.12	0.52
8:Z:356:GLN:HE21	8:Z:363:LYS:HB3	1.73	0.52
2:B:268:LYS:HD3	4:E:173:ASP:H	7.86	0.52
4:E:53:ALA:HB1	4:E:98:ASN:HD21	1.74	0.52
6:H:419:GLU:OE1	6:H:472:HIS:NE2	2.43	0.52
1:A:49:LEU:HD13	5:G:522:ARG:HA	1.92	0.52
3:D:256:ASP:OD1	3:D:257:TYR:N	2.42	0.52
2:B:115:ILE:HG21	3:D:8:ASN:HB2	39.94	0.52
8:Z:202:LEU:HD12	8:Z:381:LYS:HD2	1.90	0.52
3:D:486:ARG:HG3	3:D:490:THR:HG21	2.19	0.52
7:Q:421:PRO:O	7:Q:426:THR:OG1	2.31	0.52
1:A:53:LEU:HD21	1:A:69:ILE:HA	1.91	0.52
7:Q:238:SER:HB2	7:Q:359:LYS:HA	1.92	0.52
1:A:91:ASP:HA	1:A:95:GLY:HA2	2.13	0.52
7:Q:223:ILE:HG22	7:Q:225:GLY:H	4.41	0.52
5:G:229:VAL:HG12	5:G:231:HIS:H	1.76	0.51
8:Z:173:ILE:HG23	8:Z:209:PHE:HB2	2.28	0.51
1:A:303:ASP:OD1	1:A:304:ASP:N	2.41	0.51
2:B:342:VAL:HB	2:B:357:SER:HB3	2.54	0.51
6:H:447:GLU:OE2	6:H:469:ARG:NH2	2.48	0.51
1:A:132:ALA:HB2	1:A:448:ILE:HG12	2.02	0.51
3:D:268:ARG:HE	3:D:304:PHE:HZ	4.37	0.51
3:D:48:ILE:HD11	3:D:64:ILE:HG23	1.91	0.51
3:D:35:ILE:HG22	3:D:94:THR:HG23	2.05	0.51
3:D:354:ASP:OD1	3:D:358:SER:N	2.44	0.51
3:D:21:ARG:HD2	3:D:519:LEU:HA	1.92	0.51
6:H:391:ARG:HA	6:H:394:HIS:HD2	1.76	0.51
8:Z:68:ILE:HG21	8:Z:73:ALA:HB3	1.93	0.51
2:B:48:SER:OG	2:B:53:THR:OG1	2.27	0.51
7:Q:250:PHE:HE1	7:Q:341:LEU:HD12	6.72	0.51
8:Z:173:ILE:HG12	8:Z:209:PHE:HB2	1.92	0.51
1:A:190:GLN:HA	1:A:196:ILE:H	1.75	0.51
1:A:366:PHE:HE2	1:A:371:CYS:HB2	3.23	0.50
5:G:222:GLY:H	5:G:377:CYS:HA	1.77	0.50
6:H:104:LEU:HD11	6:H:446:LEU:HD23	1.93	0.50
5:G:69:ASP:H	8:Z:536:ALA:HB1	2.04	0.50
3:D:410:LEU:HD13	3:D:498:LEU:HD22	4.21	0.50
1:A:357:LEU:HB3	1:A:378:SER:HB3	1.93	0.50
2:B:32:LEU:HB3	2:B:44:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:243:VAL:HG21	4:E:354:ILE:HG12	3.48	0.50
6:H:519:SER:O	7:Q:51:ARG:HB3	2.11	0.50
8:Z:267:ARG:NE	8:Z:271:ASP:OD2	7.43	0.50
5:G:242:ARG:NH2	5:G:291:ARG:O	2.39	0.50
6:H:42:PRO:O	6:H:49:SER:N	2.43	0.50
6:H:77:HIS:CE1	6:H:79:ALA:HB3	2.58	0.50
2:B:118:GLN:HA	2:B:121:ILE:HD12	1.93	0.50
2:B:72:PRO:HB3	2:B:517:ALA:HB2	1.93	0.50
4:E:96:LEU:HD11	4:E:101:ALA:HB3	2.38	0.50
5:G:170:LYS:HE3	5:G:215:LEU:HD13	1.93	0.50
1:A:236:ARG:NE	1:A:360:GLU:OE2	2.42	0.50
2:B:6:PHE:HE2	2:B:515:ILE:HG12	1.76	0.50
3:D:37:THR:O	3:D:44:MET:N	2.58	0.50
3:D:411:ILE:HG21	3:D:417:PRO:HB3	4.21	0.50
5:G:223:VAL:HB	5:G:368:LEU:HD12	1.97	0.50
7:Q:511:ASP:HB3	7:Q:513:ARG:HG2	1.94	0.50
8:Z:199:MET:HG2	8:Z:201:HIS:H	5.46	0.50
1:A:170:GLY:HA2	1:A:173:SER:HB3	1.99	0.50
3:D:16:LYS:NZ	3:D:18:GLN:OE1	9.93	0.50
2:B:328:THR:HG21	4:E:182:ARG:HD3	2.63	0.50
6:H:240:LYS:HB3	6:H:346:LEU:HD22	1.93	0.50
7:Q:27:GLN:HE22	7:Q:544:ILE:H	1.59	0.50
7:Q:469:LEU:HD13	7:Q:474:VAL:HG21	2.37	0.50
3:D:335:ASP:OD1	3:D:336:ILE:N	2.45	0.50
6:H:235:LYS:HG3	6:H:351:LEU:HD11	1.94	0.50
1:A:167:LYS:HB2	1:A:169:ILE:HG22	1.95	0.49
1:A:440:VAL:HG23	1:A:441:GLY:H	4.21	0.49
5:G:110:TYR:HE2	5:G:444:ALA:HB2	1.85	0.49
4:E:112:ASP:HA	4:E:116:GLY:HA2	1.94	0.49
3:D:156:THR:HG21	3:D:496:HIS:HB3	2.39	0.49
6:H:111:GLU:HB3	6:H:441:ALA:HB1	1.95	0.49
1:A:204:ASN:OD1	1:A:205:VAL:N	3.21	0.49
2:B:142:ASN:HB2	2:B:398:THR:HG22	1.94	0.49
5:G:213:ASP:OD1	5:G:214:VAL:N	2.46	0.49
5:G:209:ILE:HG13	5:G:380:MET:HG3	3.94	0.49
7:Q:242:ASP:O	7:Q:245:HIS:NE2	2.46	0.49
4:E:278:PRO:HG3	4:E:302:GLU:HG2	2.41	0.49
3:D:72:HIS:CE1	3:D:74:VAL:HB	2.47	0.49
4:E:316:ALA:HB1	4:E:374:LEU:HD11	1.94	0.49
1:A:130:ARG:HH21	1:A:536:VAL:HG11	1.98	0.49
3:D:287:LEU:HD13	3:D:324:LEU:HD13	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:8:ASN:ND2	4:E:485:GLU:O	47.62	0.49
4:E:72:LYS:HD2	4:E:90:ILE:HD13	1.94	0.49
7:Q:203:ASN:OD1	7:Q:204:VAL:N	2.46	0.49
8:Z:233:VAL:HG11	8:Z:332:THR:HG21	1.95	0.49
8:Z:44:LYS:HD2	8:Z:62:LEU:HD13	1.95	0.49
8:Z:87:THR:HB	8:Z:512:VAL:HG22	2.31	0.49
6:H:296:LYS:HE2	6:H:320:ALA:HA	2.67	0.48
6:H:480:GLY:HA3	6:H:491:ASN:HD22	1.77	0.48
7:Q:92:GLN:NE2	7:Q:98:ASP:O	3.57	0.48
8:Z:301:ILE:HB	8:Z:318:ARG:HD3	1.94	0.48
8:Z:12:SER:OG	8:Z:532:GLU:OE2	2.31	0.48
1:A:406:LEU:HB3	1:A:410:LYS:HE3	6.61	0.48
1:A:58:GLY:O	5:G:76:LYS:NZ	2.45	0.48
4:E:167:ASP:OD1	4:E:168:ILE:N	4.72	0.48
4:E:328:ASP:OD1	4:E:329:ASP:N	2.43	0.48
7:Q:43:LEU:HD23	7:Q:105:ILE:HG12	1.95	0.48
8:Z:119:THR:HG23	8:Z:525:SER:HB3	1.94	0.48
1:A:206:LEU:HD12	1:A:386:ILE:HG12	1.94	0.48
6:H:143:LEU:HD21	6:H:419:GLU:HG2	1.95	0.48
8:Z:212:GLY:N	8:Z:368:THR:HG22	2.24	0.48
3:D:226:PRO:O	3:D:227:THR:OG1	2.29	0.48
3:D:500:PRO:HG2	3:D:503:VAL:HG23	1.97	0.48
3:D:29:ARG:NH1	3:D:108:GLU:OE1	2.46	0.48
4:E:245:LEU:HD22	4:E:354:ILE:HD11	1.96	0.48
7:Q:98:ASP:OD1	7:Q:99:GLY:N	2.44	0.48
2:B:85:ASP:OD1	2:B:92:THR:OG1	2.31	0.48
3:D:103:LEU:HB2	3:D:515:VAL:HG21	2.02	0.48
3:D:211:ASP:HA	3:D:375:VAL:HG13	1.95	0.48
4:E:107:LEU:HD11	4:E:540:LEU:HB3	2.15	0.48
6:H:201:ILE:HD12	6:H:390:GLU:HG3	3.03	0.48
7:Q:291:ILE:HA	7:Q:347:PRO:HG3	2.09	0.48
8:Z:35:THR:O	8:Z:42:THR:N	3.23	0.48
1:A:59:ASP:OD1	1:A:60:PHE:N	2.43	0.48
2:B:459:LEU:HD22	2:B:472:LEU:HG	2.82	0.48
3:D:228:ARG:HE	3:D:349:LEU:HD11	1.79	0.48
2:B:116:HIS:NE2	4:E:486:ASN:O	5.58	0.48
5:G:110:TYR:HD1	5:G:114:LYS:HG3	1.90	0.48
6:H:285:VAL:HG13	6:H:290:ALA:HB3	2.21	0.48
7:Q:155:ASP:OD1	7:Q:156:LYS:N	2.47	0.48
1:A:322:LYS:HE2	1:A:324:GLU:HB2	1.94	0.48
8:Z:39:PRO:HA	8:Z:160:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:244:PRO:HD2	3:D:267:GLU:HG2	2.97	0.48
4:E:64:SER:HA	4:E:70:LEU:H	2.56	0.48
5:G:471:LEU:HD22	5:G:484:ILE:HD11	1.96	0.48
2:B:455:LEU:HB3	2:B:472:LEU:HD22	3.68	0.48
3:D:293:LEU:HG	3:D:294:ARG:HG2	3.49	0.48
1:A:546:THR:HA	3:D:49:LYS:HB3	2.16	0.48
1:A:133:LEU:HD22	1:A:532:LEU:HD22	1.96	0.47
1:A:94:ILE:HD11	1:A:526:LYS:HB2	1.96	0.47
7:Q:32:ILE:HG12	7:Q:111:LEU:HB3	1.96	0.47
8:Z:195:GLU:OE2	8:Z:327:ARG:NE	2.94	0.47
5:G:129:LEU:HD12	5:G:514:ILE:HB	1.96	0.47
2:B:45:LEU:HD23	3:D:524:ILE:HG23	8.79	0.47
4:E:250:SER:OG	4:E:332:ASN:ND2	2.48	0.47
8:Z:98:VAL:HG13	8:Z:524:ALA:HB2	1.96	0.47
3:D:91:ASP:OD1	3:D:92:GLY:N	2.47	0.47
4:E:212:MET:HB3	4:E:219:VAL:HG22	3.14	0.47
5:G:296:ILE:HG12	5:G:317:LEU:HD23	2.09	0.47
5:G:221:LYS:N	5:G:369:ASP:OD1	7.19	0.47
8:Z:239:SER:HB2	8:Z:299:LYS:HD3	1.96	0.47
1:A:462:LEU:HB3	1:A:504:LEU:HD21	5.24	0.47
2:B:400:THR:HG22	2:B:490:SER:HA	1.96	0.47
1:A:183:ALA:O	1:A:187:VAL:HG23	2.15	0.47
2:B:244:LYS:HB2	4:E:209:ILE:HG22	3.63	0.47
5:G:454:ARG:NH2	7:Q:120:MET:O	55.46	0.47
7:Q:91:GLN:HE21	8:Z:383:SER:HB2	1.79	0.47
8:Z:89:ASP:OD1	8:Z:90:GLY:N	2.49	0.47
3:D:197:VAL:HB	3:D:378:VAL:HA	1.97	0.47
3:D:358:SER:OG	3:D:380:ARG:NH1	2.44	0.47
6:H:329:ALA:HA	6:H:371:ALA:HA	1.99	0.47
8:Z:198:GLN:HE21	8:Z:388:LEU:HD13	3.43	0.47
4:E:111:GLN:O	4:E:116:GLY:N	2.48	0.47
5:G:241:PRO:HG2	5:G:352:CYS:HB3	1.96	0.47
1:A:326:LEU:HA	1:A:329:ILE:HD12	1.96	0.47
1:A:419:VAL:HG21	1:A:524:LYS:HG3	4.10	0.47
4:E:160:LYS:HG3	4:E:453:ALA:HB1	1.97	0.47
4:E:182:ARG:HH12	4:E:526:PHE:HD2	1.63	0.47
6:H:181:MET:HG2	6:H:214:PHE:HB2	1.97	0.47
7:Q:16:GLN:HB2	7:Q:18:TYR:HE2	1.80	0.47
7:Q:341:LEU:HD12	7:Q:342:PRO:HD2	1.96	0.47
2:B:27:ILE:O	2:B:31:ASP:N	2.48	0.47
2:B:216:LYS:HE3	2:B:308:HIS:HD2	7.04	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:180:LEU:HG	4:E:430:VAL:HG22	1.97	0.47
8:Z:183:ASP:OD1	8:Z:184:ALA:N	4.73	0.47
8:Z:207:THR:HA	8:Z:381:LYS:HD2	6.00	0.47
3:D:317:GLU:HG3	3:D:319:GLU:H	1.80	0.46
3:D:461:ASN:HB3	3:D:464:LYS:HB3	1.97	0.46
4:E:229:ARG:HG3	4:E:392:MET:HE3	4.76	0.46
3:D:99:LEU:HB2	3:D:450:ILE:HD11	2.22	0.46
4:E:397:GLN:HG3	4:E:399:LYS:H	1.80	0.46
6:H:37:GLN:HE22	6:H:107:GLU:HB2	1.80	0.46
2:B:213:ILE:HB	2:B:366:THR:HG21	1.96	0.46
2:B:276:ILE:HG23	2:B:281:ILE:HD11	1.97	0.46
5:G:454:ARG:HB2	5:G:468:LEU:HD11	3.90	0.46
1:A:104:ILE:HG13	1:A:458:ILE:HD11	1.97	0.46
4:E:267:VAL:HG21	4:E:379:ARG:HA	2.07	0.46
5:G:110:TYR:HB3	5:G:116:ILE:HD12	2.23	0.46
6:H:244:LEU:HB2	6:H:295:SER:HB2	4.16	0.46
7:Q:373:GLN:HE22	7:Q:379:SER:H	1.62	0.46
7:Q:27:GLN:NE2	7:Q:544:ILE:HG12	2.29	0.46
8:Z:158:LEU:O	8:Z:162:VAL:HG22	2.16	0.46
3:D:72:HIS:HE1	3:D:74:VAL:HB	1.80	0.46
8:Z:245:THR:HG22	8:Z:247:VAL:H	1.80	0.46
1:A:20:ILE:HG22	1:A:25:ILE:HB	6.12	0.46
2:B:423:ASP:OD1	2:B:424:GLY:N	2.41	0.46
4:E:326:GLY:HA2	4:E:344:ARG:HE	4.56	0.46
1:A:156:LEU:HD11	1:A:413:LEU:HD21	1.97	0.46
2:B:511:VAL:HG13	2:B:513:ASN:O	2.94	0.46
4:E:303:GLN:HE21	4:E:334:LEU:HD21	1.81	0.46
2:B:112:GLN:HG2	3:D:12:LYS:HD2	18.87	0.46
7:Q:15:LYS:O	8:Z:69:GLN:N	2.44	0.46
2:B:189:ASN:OD1	2:B:190:LEU:N	2.49	0.46
2:B:341:ASP:HB2	2:B:358:GLY:HA3	1.98	0.46
2:B:510:ARG:NH2	4:E:69:GLY:O	9.65	0.46
7:Q:413:LYS:O	7:Q:415:SER:N	2.47	0.46
1:A:39:VAL:O	1:A:51:LYS:NZ	2.44	0.46
4:E:502:GLN:HE21	4:E:510:ILE:H	1.79	0.45
5:G:246:LEU:HD11	5:G:297:THR:HG23	2.42	0.45
6:H:242:LEU:HD21	6:H:341:ILE:HD13	2.36	0.45
6:H:299:ILE:HD13	6:H:314:CYS:HB2	2.17	0.45
8:Z:234:LEU:HD13	8:Z:348:LEU:HD23	2.05	0.45
1:A:96:ASP:OD1	1:A:97:GLY:N	2.50	0.45
3:D:180:LYS:NZ	3:D:211:ASP:OD2	6.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:189:LEU:HD21	8:Z:403:ALA:HA	1.97	0.45
7:Q:255:ASP:OD1	7:Q:256:ILE:N	2.47	0.45
8:Z:184:ALA:O	8:Z:185:GLN:HG3	4.58	0.45
1:A:443:ARG:HH22	3:D:461:ASN:HB2	1.81	0.45
2:B:201:GLY:HA3	2:B:370:ARG:HD3	3.73	0.45
2:B:172:HIS:NE2	2:B:206:SER:O	2.41	0.45
5:G:295:VAL:HG21	5:G:309:LEU:HD13	1.99	0.45
1:A:248:ASP:HB2	1:A:337:LEU:HD11	1.97	0.45
1:A:37:ALA:O	1:A:41:LYS:HG3	4.60	0.45
1:A:512:GLU:HA	1:A:515:ALA:HB3	1.98	0.45
3:D:117:PRO:HA	3:D:120:ILE:HD12	1.98	0.45
5:G:334:ALA:HA	5:G:347:ASP:HA	2.63	0.45
6:H:155:ARG:O	6:H:159:GLU:N	2.42	0.45
6:H:519:SER:HA	7:Q:51:ARG:HD2	1.97	0.45
8:Z:106:HIS:HA	8:Z:109:ILE:HD12	2.53	0.45
1:A:208:ALA:HB3	1:A:388:ARG:HG2	1.99	0.45
1:A:394:SER:O	1:A:398:MET:N	2.76	0.45
3:D:434:GLY:HA2	4:E:493:GLY:HA2	63.06	0.45
1:A:74:ASP:HB3	5:G:529:GLY:HA3	3.44	0.45
6:H:224:PHE:HZ	6:H:315:ALA:HA	1.87	0.45
6:H:292:ILE:HD13	6:H:313:PHE:HB3	2.37	0.45
6:H:342:LYS:H	6:H:345:HIS:HD2	1.64	0.45
3:D:372:ARG:O	3:D:374:THR:N	2.50	0.45
7:Q:46:MET:HB2	7:Q:101:ASN:HB3	2.02	0.45
8:Z:251:PHE:HB3	8:Z:262:LEU:HB3	4.24	0.45
1:A:285:VAL:HG21	1:A:306:CYS:HB3	1.98	0.45
3:D:241:ILE:HD12	3:D:297:VAL:HG22	3.71	0.45
5:G:411:SER:OG	5:G:503:GLU:OE1	2.32	0.45
7:Q:292:ALA:HB2	7:Q:318:ILE:HD11	1.98	0.45
8:Z:531:ASP:OD1	8:Z:532:GLU:N	2.49	0.45
2:B:229:ALA:HA	2:B:282:ASN:HD21	1.90	0.45
3:D:46:LYS:HD2	3:D:64:ILE:HG21	2.34	0.45
7:Q:150:ILE:HB	7:Q:417:GLY:HA2	2.16	0.45
7:Q:208:ARG:NH2	7:Q:328:GLU:OE2	2.67	0.45
8:Z:75:LEU:HG	8:Z:523:ILE:HG23	6.11	0.45
5:G:160:GLY:O	5:G:161:THR:OG1	2.32	0.45
5:G:356:LYS:HG2	5:G:358:GLU:H	4.95	0.45
6:H:288:THR:HG22	6:H:346:LEU:HD11	5.39	0.45
7:Q:190:LEU:HD21	7:Q:202:PHE:HB2	2.24	0.45
8:Z:86:ILE:HG23	8:Z:511:ARG:HH21	8.82	0.45
3:D:163:VAL:HG12	3:D:204:ILE:HD13	4.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:164:VAL:HB	5:G:171:MET:HG3	1.97	0.44
5:G:44:MET:HG2	8:Z:529:LEU:HD22	3.03	0.44
7:Q:343:ARG:NH2	8:Z:253:TYR:O	7.94	0.44
1:A:49:LEU:HB3	5:G:522:ARG:O	2.51	0.44
1:A:200:VAL:HA	1:A:410:LYS:HD2	1.99	0.44
4:E:377:CYS:HA	4:E:397:GLN:NE2	3.17	0.44
4:E:96:LEU:HD13	4:E:98:ASN:HB3	1.99	0.44
5:G:82:SER:HB3	5:G:97:ILE:HD11	2.86	0.44
5:G:243:VAL:HG22	5:G:294:LEU:HD23	6.11	0.44
7:Q:130:GLY:HA3	7:Q:448:ALA:HB3	2.26	0.44
1:A:19:LYS:HE2	1:A:543:THR:HG21	2.06	0.44
3:D:16:LYS:HD3	3:D:19:GLU:HG3	1.98	0.44
3:D:237:ILE:HD11	3:D:286:LEU:HD22	2.00	0.44
3:D:368:ASN:OD1	3:D:369:ASN:N	2.50	0.44
3:D:70:ILE:HG21	3:D:75:ALA:HB3	2.11	0.44
5:G:301:VAL:HG23	5:G:318:ARG:HB3	2.11	0.44
6:H:177:PHE:HD2	6:H:210:GLU:HB2	1.82	0.44
7:Q:242:ASP:OD1	7:Q:243:LYS:N	2.65	0.44
3:D:284:ASN:HA	3:D:310:ILE:HG12	3.27	0.44
1:A:78:PRO:HB3	3:D:55:ILE:HD13	4.93	0.44
4:E:326:GLY:HA2	4:E:344:ARG:HB2	1.99	0.44
5:G:156:GLN:HA	5:G:159:ILE:HD12	4.90	0.44
4:E:282:LYS:HA	4:E:285:HIS:CE1	3.46	0.44
5:G:243:VAL:N	5:G:349:GLY:HA3	2.29	0.44
5:G:44:MET:HB3	8:Z:529:LEU:O	2.18	0.44
7:Q:541:ILE:HD11	8:Z:55:LEU:HD21	2.33	0.44
1:A:437:ALA:HB1	1:A:445:GLN:HG3	1.99	0.43
3:D:423:ARG:HH12	4:E:466:GLN:HE22	105.38	0.43
6:H:248:LEU:HB3	6:H:299:ILE:HG23	1.99	0.43
7:Q:428:ILE:HD13	7:Q:478:LEU:HB3	4.89	0.43
8:Z:11:GLU:H	8:Z:535:ARG:HB3	1.83	0.43
2:B:84:GLN:HE22	2:B:496:ALA:HB1	2.37	0.43
5:G:14:ARG:HG2	5:G:527:VAL:HA	3.66	0.43
1:A:73:LEU:HG	1:A:75:VAL:HG23	2.00	0.43
6:H:335:GLN:HG2	6:H:341:ILE:HA	2.00	0.43
7:Q:348:THR:HG22	7:Q:350:GLU:H	1.83	0.43
1:A:480:TYR:HB3	1:A:500:TYR:HD2	1.82	0.43
2:B:514:ILE:HG12	4:E:73:ILE:HD12	2.00	0.43
3:D:283:CYS:SG	3:D:344:LEU:HD11	2.59	0.43
6:H:454:CYS:HB3	6:H:459:PHE:HB2	2.13	0.43
7:Q:390:THR:HG22	7:Q:393:ASN:H	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:280:LEU:HD21	8:Z:348:LEU:HD21	2.24	0.43
8:Z:423:SER:HB2	8:Z:451:LEU:HB2	2.35	0.43
3:D:333:ILE:HG21	3:D:339:PHE:HB2	2.01	0.43
8:Z:437:LYS:HB3	8:Z:440:THR:HB	2.85	0.43
1:A:191:ASN:ND2	1:A:197:LYS:HB2	3.61	0.43
1:A:144:LEU:HD22	1:A:417:ASN:HD21	3.84	0.43
1:A:480:TYR:HB3	1:A:500:TYR:CD2	2.54	0.43
2:B:230:LYS:HB2	2:B:281:ILE:HA	2.07	0.43
2:B:290:ILE:HD13	2:B:298:PHE:HE2	1.83	0.43
2:B:237:THR:OG1	4:E:177:ARG:NH1	2.50	0.43
4:E:225:LYS:HB2	4:E:405:THR:HA	3.66	0.43
5:G:424:SER:HB3	5:G:449:MET:HB2	2.00	0.43
6:H:40:LEU:HB3	6:H:99:THR:HG23	2.16	0.43
7:Q:27:GLN:HE22	7:Q:544:ILE:N	2.16	0.43
8:Z:189:LEU:HG	8:Z:407:LYS:HE3	2.00	0.43
2:B:35:SER:O	2:B:447:ASN:ND2	3.31	0.43
5:G:295:VAL:N	5:G:315:SER:O	2.47	0.43
7:Q:244:LYS:H	7:Q:356:GLU:HA	1.84	0.43
8:Z:122:PHE:HB3	8:Z:521:THR:HG23	2.22	0.43
1:A:140:ILE:O	1:A:144:LEU:HG	2.18	0.43
3:D:350:VAL:HG22	3:D:363:VAL:HG22	2.04	0.43
3:D:85:GLN:HB3	3:D:93:THR:HG22	1.99	0.43
4:E:58:ALA:O	4:E:62:LYS:HG3	2.25	0.43
8:Z:57:LYS:HD2	8:Z:161:LYS:HA	2.01	0.43
1:A:462:LEU:HG	1:A:504:LEU:HD11	2.00	0.43
2:B:512:ASP:OD1	2:B:513:ASN:N	2.51	0.43
3:D:403:CYS:HB3	3:D:502:LEU:HB3	2.01	0.43
6:H:512:GLU:OE2	7:Q:393:ASN:ND2	2.51	0.43
7:Q:362:GLU:HB2	7:Q:367:ARG:NH1	2.34	0.43
3:D:214:VAL:HG11	3:D:378:VAL:HG22	2.26	0.43
5:G:339:ARG:HG2	5:G:341:GLU:H	1.83	0.43
5:G:454:ARG:HD2	5:G:468:LEU:HD22	2.01	0.43
1:A:51:LYS:HA	5:G:523:VAL:HG13	2.44	0.43
6:H:232:GLN:HG2	6:H:308:ALA:HA	3.20	0.43
1:A:302:ILE:H	1:A:319:ARG:HG2	1.92	0.42
1:A:133:LEU:HD22	1:A:532:LEU:HD23	3.13	0.42
2:B:218:PHE:HB2	2:B:306:ILE:HA	2.01	0.42
2:B:320:VAL:HG23	2:B:321:THR:HG23	2.21	0.42
5:G:139:VAL:HG22	5:G:480:PHE:HD2	1.84	0.42
5:G:331:VAL:HG12	5:G:374:PRO:HG2	2.80	0.42
7:Q:294:MET:HG3	7:Q:347:PRO:HG2	3.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ASP:HB2	4:E:177:ARG:HD3	9.09	0.42
3:D:116:HIS:CG	3:D:117:PRO:HD2	2.54	0.42
5:G:417:GLY:HA3	5:G:453:PRO:HB3	2.01	0.42
5:G:63:ALA:HA	5:G:66:ARG:HH21	1.83	0.42
6:H:37:GLN:O	6:H:41:LYS:HG3	2.20	0.42
1:A:404:ASP:O	1:A:407:SER:OG	2.29	0.42
2:B:14:ARG:NH1	2:B:16:GLU:HB3	2.33	0.42
3:D:178:VAL:HA	3:D:181:ILE:HG12	2.00	0.42
3:D:226:PRO:HG3	3:D:311:MET:HA	2.01	0.42
5:G:204:VAL:HG12	5:G:204:VAL:O	2.19	0.42
7:Q:362:GLU:HA	7:Q:367:ARG:HA	2.69	0.42
8:Z:189:LEU:HD11	8:Z:403:ALA:HB1	2.10	0.42
4:E:334:LEU:O	4:E:338:ASN:ND2	2.41	0.42
7:Q:38:LEU:HD12	7:Q:82:VAL:HG11	2.02	0.42
8:Z:294:VAL:HG13	8:Z:315:LEU:HB3	2.01	0.42
1:A:164:MET:HB3	1:A:169:ILE:HG23	2.02	0.42
1:A:207:LYS:HB2	1:A:395:LEU:HB3	3.30	0.42
3:D:213:VAL:HG11	3:D:328:LEU:HD21	2.02	0.42
4:E:68:ARG:HD2	4:E:487:SER:HA	3.02	0.42
1:A:94:ILE:HD11	1:A:522:ILE:HG22	3.38	0.42
5:G:379:ILE:HD13	5:G:396:LEU:HD21	2.55	0.42
6:H:94:VAL:HG12	6:H:96:ASP:H	1.91	0.42
5:G:454:ARG:HH12	7:Q:120:MET:HG3	61.98	0.42
4:E:142:HIS:CD2	6:H:458:GLY:HA2	2.55	0.42
7:Q:258:ASN:O	8:Z:253:TYR:OH	2.33	0.42
4:E:246:ASP:HA	4:E:392:MET:HG2	3.90	0.42
7:Q:18:TYR:HB3	7:Q:547:ALA:HA	3.46	0.42
8:Z:221:HIS:CG	8:Z:222:PRO:HD2	2.64	0.42
1:A:51:LYS:HD2	1:A:69:ILE:HG21	4.12	0.42
2:B:410:VAL:HA	2:B:413:LYS:HE2	2.01	0.42
2:B:98:LEU:HD13	2:B:440:LEU:HD11	2.00	0.42
3:D:243:PRO:HD3	3:D:298:ASN:HD22	1.85	0.42
4:E:381:TYR:HE1	4:E:383:GLN:HB2	1.85	0.42
5:G:354:LEU:HD13	5:G:356:LYS:HB3	5.32	0.42
7:Q:500:ASP:OD1	7:Q:501:ILE:N	2.52	0.42
8:Z:115:PRO:HA	8:Z:118:ILE:HD12	2.46	0.42
8:Z:207:THR:OG1	8:Z:379:LEU:O	4.29	0.42
8:Z:490:GLY:O	8:Z:499:CYS:N	2.52	0.42
1:A:121:HIS:CG	1:A:122:PRO:HD2	2.56	0.42
4:E:99:GLU:HB3	6:H:52:LEU:HD22	2.02	0.42
6:H:410:VAL:HG21	6:H:503:LYS:HD2	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:HD2	1:A:454:ALA:HB2	2.01	0.41
1:A:219:VAL:O	1:A:383:SER:OG	2.29	0.41
2:B:217:LYS:HA	2:B:354:LEU:HD21	2.02	0.41
2:B:157:ALA:HB2	2:B:391:LEU:HD11	2.02	0.41
3:D:178:VAL:HG11	3:D:401:ILE:HG22	2.10	0.41
6:H:476:GLU:HB3	6:H:479:TYR:CZ	2.95	0.41
7:Q:93:LYS:NZ	7:Q:403:ASP:OD1	2.56	0.41
8:Z:187:ASP:HB3	8:Z:188:ASN:H	2.05	0.41
1:A:173:SER:HA	1:A:176:PHE:HB2	2.03	0.41
3:D:195:ARG:O	3:D:377:VAL:N	2.51	0.41
3:D:420:GLU:OE1	3:D:473:HIS:NE2	6.51	0.41
8:Z:23:VAL:HG13	8:Z:102:LEU:HB3	2.02	0.41
4:E:256:LYS:HB3	4:E:382:GLU:HB3	2.55	0.41
1:A:258:MET:HB3	5:G:344:LYS:HA	2.02	0.41
5:G:465:ILE:HG22	7:Q:444:LEU:HD22	60.70	0.41
8:Z:215:LEU:HG	8:Z:365:THR:HB	4.03	0.41
1:A:440:VAL:HG23	1:A:441:GLY:N	4.55	0.41
3:D:18:GLN:HG2	3:D:21:ARG:HH22	1.86	0.41
3:D:239:PHE:CG	3:D:240:GLN:N	2.88	0.41
3:D:515:VAL:HA	3:D:518:ILE:HD12	2.49	0.41
6:H:198:LEU:HD22	6:H:373:THR:HB	3.07	0.41
6:H:465:LEU:HD11	6:H:469:ARG:HH22	5.84	0.41
7:Q:335:VAL:HG13	7:Q:379:SER:HB2	2.38	0.41
1:A:188:LYS:HB3	1:A:198:TYR:CE1	2.55	0.41
3:D:173:LEU:HD22	3:D:207:THR:HG21	2.03	0.41
4:E:385:PHE:HZ	4:E:394:ILE:HD11	2.00	0.41
5:G:414:PRO:HG3	5:G:481:THR:HA	2.02	0.41
6:H:229:PHE:CG	6:H:230:GLU:N	2.89	0.41
6:H:178:PHE:HB3	6:H:393:LEU:HD21	2.47	0.41
6:H:21:GLN:HE21	6:H:524:ILE:HG12	9.81	0.41
8:Z:185:GLN:HE21	8:Z:187:ASP:HB2	1.85	0.41
1:A:176:PHE:HZ	1:A:213:ALA:HB1	1.85	0.41
1:A:460:LYS:HG3	1:A:470:SER:HB2	2.55	0.41
2:B:326:VAL:HG22	2:B:328:THR:H	1.85	0.41
3:D:72:HIS:O	3:D:76:ARG:HG3	2.21	0.41
8:Z:114:HIS:CG	8:Z:115:PRO:HD2	2.58	0.41
2:B:196:ILE:HB	2:B:368:VAL:HG22	2.03	0.41
2:B:68:PRO:HD3	3:D:528:ARG:H	1.85	0.41
4:E:71:ASP:OD1	4:E:85:ASN:HB3	2.21	0.41
4:E:98:ASN:O	4:E:102:LYS:HG3	2.19	0.41
6:H:322:ASP:O	6:H:326:VAL:HG23	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:342:LYS:HB2	6:H:345:HIS:CD2	2.55	0.41
2:B:449:GLY:HA2	3:D:116:HIS:CG	2.55	0.41
2:B:5:ILE:HA	4:E:96:LEU:HB3	2.49	0.41
5:G:117:HIS:CG	5:G:118:PRO:HD2	2.56	0.41
7:Q:349:PRO:HA	7:Q:352:LEU:HD12	2.01	0.41
7:Q:71:MET:HE2	7:Q:75:LEU:HD11	6.92	0.41
8:Z:301:ILE:HG13	8:Z:318:ARG:HB3	2.03	0.41
1:A:366:PHE:HB2	1:A:369:ASP:HB3	5.90	0.41
3:D:81:VAL:HG13	3:D:510:LEU:HB3	2.02	0.41
4:E:249:PHE:HE1	4:E:393:LEU:HD22	1.86	0.41
4:E:46:ALA:HB1	4:E:50:HIS:CE1	2.56	0.41
5:G:330:ARG:NH2	5:G:374:PRO:O	2.54	0.41
6:H:461:ALA:HA	6:H:464:ILE:HG22	2.03	0.41
7:Q:170:LYS:HG2	7:Q:171:LYS:HG2	2.03	0.41
8:Z:328:LEU:O	8:Z:332:THR:OG1	2.24	0.41
1:A:482:ALA:O	1:A:486:MET:HG3	2.21	0.41
1:A:7:ASN:OD1	1:A:8:SER:N	2.86	0.41
2:B:244:LYS:HD2	4:E:400:GLU:HB2	6.24	0.41
2:B:427:SER:HG	2:B:457:SER:HG	22.37	0.41
3:D:196:LEU:HD22	3:D:379:ILE:HD11	2.03	0.41
4:E:517:TYR:CG	4:E:518:GLY:N	4.29	0.41
4:E:74:LEU:HD11	4:E:90:ILE:HG12	2.12	0.41
1:A:465:ASN:HA	5:G:117:HIS:HE2	2.59	0.41
6:H:96:ASP:OD1	6:H:97:GLY:N	2.54	0.41
1:A:73:LEU:HD13	5:G:527:VAL:HG13	2.01	0.41
2:B:41:GLY:HA2	2:B:447:ASN:HB3	2.03	0.41
5:G:64:ILE:O	5:G:68:ILE:HG12	3.88	0.41
3:D:469:LEU:HD11	3:D:482:ILE:HG13	2.28	0.40
3:D:516:LYS:O	3:D:520:ARG:HG3	2.38	0.40
5:G:145:VAL:HG11	5:G:196:PHE:HE2	5.43	0.40
5:G:210:PRO:HA	5:G:389:LEU:HD11	2.53	0.40
2:B:105:GLU:HB3	2:B:432:ALA:HB1	2.03	0.40
4:E:245:LEU:HD11	4:E:346:VAL:HG22	2.04	0.40
4:E:249:PHE:CE2	4:E:382:GLU:HB2	2.66	0.40
4:E:510:ILE:HG12	4:E:521:ASP:HA	2.11	0.40
6:H:67:ALA:HB2	6:H:98:THR:HG21	2.03	0.40
8:Z:187:ASP:CG	8:Z:188:ASN:H	2.24	0.40
4:E:142:HIS:CG	4:E:143:PRO:HD2	2.57	0.40
5:G:188:GLN:HE21	5:G:191:GLU:H	1.70	0.40
8:Z:235:ILE:HD13	8:Z:296:ILE:HG13	2.03	0.40
3:D:492:THR:HB	3:D:497:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:351:LEU:HD23	4:E:354:ILE:HD12	2.03	0.40
5:G:140:SER:HB3	5:G:411:SER:HB2	2.14	0.40
5:G:24:ASN:ND2	5:G:523:VAL:O	2.54	0.40
8:Z:323:ARG:HG3	8:Z:327:ARG:NH1	2.35	0.40
8:Z:359:ILE:HB	8:Z:362:GLU:O	2.21	0.40
3:D:191:LEU:HD22	3:D:398:LEU:HB3	2.03	0.40
4:E:378:SER:HB3	4:E:397:GLN:O	2.21	0.40
6:H:357:ILE:HG23	6:H:379:ARG:HD2	2.02	0.40
6:H:201:ILE:HG21	6:H:390:GLU:HG3	2.03	0.40
7:Q:141:GLU:O	7:Q:145:MET:HG2	2.22	0.40
7:Q:506:ASP:OD1	7:Q:507:GLU:HG3	2.21	0.40
8:Z:492:ASP:HB2	8:Z:499:CYS:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	541/559 (97%)	506 (94%)	35 (6%)	0	100	100
1	a	541/559 (97%)	511 (94%)	29 (5%)	1 (0%)	52	86
2	B	515/527 (98%)	490 (95%)	25 (5%)	0	100	100
2	b	515/527 (98%)	488 (95%)	26 (5%)	1 (0%)	52	86
3	D	519/528 (98%)	496 (96%)	21 (4%)	2 (0%)	39	80
3	d	519/528 (98%)	495 (95%)	22 (4%)	2 (0%)	39	80
4	E	526/562 (94%)	502 (95%)	24 (5%)	0	100	100
4	e	526/562 (94%)	505 (96%)	21 (4%)	0	100	100
5	G	516/534 (97%)	497 (96%)	19 (4%)	0	100	100
5	g	516/534 (97%)	495 (96%)	20 (4%)	1 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	517/550 (94%)	501 (97%)	15 (3%)	1 (0%)	52	86
6	h	517/550 (94%)	501 (97%)	16 (3%)	0	100	100
7	Q	541/568 (95%)	518 (96%)	23 (4%)	0	100	100
7	q	541/568 (95%)	516 (95%)	25 (5%)	0	100	100
8	Z	532/546 (97%)	512 (96%)	20 (4%)	0	100	100
8	z	532/546 (97%)	514 (97%)	18 (3%)	0	100	100
All	All	8414/8748 (96%)	8047 (96%)	359 (4%)	8 (0%)	59	90

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	H	245	ASN
5	g	195	ASN
3	d	213	VAL
3	D	213	VAL
2	b	467	ILE
1	a	203	VAL
3	d	210	ILE
3	D	210	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	455/471 (97%)	455 (100%)	0	100	100
1	a	455/471 (97%)	455 (100%)	0	100	100
2	B	432/441 (98%)	432 (100%)	0	100	100
2	b	432/441 (98%)	432 (100%)	0	100	100
3	D	447/453 (99%)	447 (100%)	0	100	100
3	d	447/453 (99%)	447 (100%)	0	100	100
4	E	454/483 (94%)	454 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	e	454/483 (94%)	454 (100%)	0	100	100
5	G	441/455 (97%)	441 (100%)	0	100	100
5	g	441/455 (97%)	441 (100%)	0	100	100
6	H	432/454 (95%)	432 (100%)	0	100	100
6	h	432/454 (95%)	432 (100%)	0	100	100
7	Q	454/473 (96%)	454 (100%)	0	100	100
7	q	454/473 (96%)	454 (100%)	0	100	100
8	Z	451/463 (97%)	451 (100%)	0	100	100
8	z	451/463 (97%)	451 (100%)	0	100	100
All	All	7132/7386 (97%)	7132 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	89	GLN
1	a	90	GLN
1	a	209	HIS
2	b	222	GLN
2	b	308	HIS
2	b	447	ASN
2	B	393	GLN
3	d	250	ASN
3	d	289	GLN
3	D	250	ASN
3	D	284	ASN
3	D	289	GLN
4	e	142	HIS
4	e	432	ASN
4	e	466	GLN
4	e	502	GLN
4	e	536	GLN
4	E	303	GLN
4	E	332	ASN
4	E	536	GLN
5	G	85	GLN
5	G	188	GLN
6	H	37	GLN

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Mol	Chain	Res	Type
6	H	356	GLN
6	H	394	HIS
6	H	491	ASN
7	Q	27	GLN
7	Q	129	GLN
7	Q	373	GLN
8	z	198	GLN
8	z	385	HIS
8	Z	185	GLN
8	Z	297	ASN
8	Z	356	GLN
8	Z	385	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.